STATISTICAL MECHANICS OF COLLISIONLESS ORBITS. I. ORIGIN OF CENTRAL CUSPS IN DARK-MATTER HALOS

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ABSTRACT

We present an equilibrium statistical mechanical theory of collisionless self-gravitational systems with isotropic velocity distributions. Compared to existing standard theories, we introduce two changes: (1) the number of possible microstates is computed in energy (orbit) space rather than phase space and (2) low occupation numbers are treated more appropriately than using Stirling's approximation. Combined, the two modifications predict that the relaxed parts of collisionless self-gravitating systems, such as dark-matter halos, have a differential energy distribution $N(\varepsilon) \propto [\exp(\phi_0 - \varepsilon) - 1]$, dubbed "DARKexp". Such systems have central power-law density cusps $\rho(r) \propto r^{-1}$, which suggests a statistical mechanical origin of cusps in simulated dark-matter halos.

Subject headings: dark matter — galaxies: halos — galaxies: kinematics and dynamics — methods: analytical

1. INTRODUCTION

The apparent universal light distributions in elliptical galaxies with two-body collision relaxation time exceeding the age of the universe motivated Ogorodnikov (1957) and Lynden-Bell (1967) to seek a fast relaxation process driving the systems toward equilibrium in a statistical mechanical sense. In a seminal paper, Lynden-Bell (1967) introduced the process of 'violent relaxation' (collective energy exchange between rapid potential fluctuations and individual particles) as responsible for a short time scale for relaxation. In the same paper, he introduced a new kind of statistical mechanics, that of distinguishable particles subject to an exclusion principle because collisionless dynamics precludes two parcels of phase space from being superimposed. In the non-degenerate limit the theory predicts that isothermal spheres are the maximum entropy equilibrium states of the process, as also found by Ogorodnikov (1957).

The predictions of the theory are, however, not entirely satisfactory. It predicts infinite mass systems despite being derived under the constraints of fixed energy and mass. It also predicts mass (phase-space density) segregation despite the dynamics being collisionless (i.e., mass independent; Severne & Luwel 1986; Hjorth & Madsen 1993; Nakamura 2000; Arad & Lynden-Bell 2005; Arad & Johansson 2005). The resulting isothermal sphere profile does not reproduce the light profiles of elliptical galaxies which was the original motivation. There is an arbitrariness in defining the initial states and whether to use a particle or phase element approach (Shu 1978; Madsen 1987; Shu 1987; Hjorth & Madsen 1993; Kull et al. 1996, 1997; Bindoni & Secco 2008), which makes it difficult to assess whether the degenerate limit may be relevant. And finally, it is not obvious how to

extend the statistical mechanical approach to (spherical) systems with anisotropic velocity distributions.

Some of these issues have been addressed in terms of modifications of the extent of the relaxation process, so-called incomplete violent relaxation (Stiavelli & Bertin 1987), relaxation in a finite volume (Hjorth & Madsen 1991), or explicit scattering processes (Spergel & Hernquist 1992). Another approach has been to propose a change in the entropy functional to be optimized, applicable to non-extensive systems (Tsallis 1988; Plastino & Plastino 1993), although this has been demonstrated not to work (Barnes et al. 2007; Féron & Hjorth 2008).

To address the infinite-mass problem, Madsen (1996) (and later Menon et al. 2006; Dubey et al. 2008) showed that appropriately dealing with small occupation numbers leads to finite-mass systems, similar to King (1966) models, suitable for the description of globular clusters, which are driven by collisional relaxation.

The subject of the origin of universal collisionless self-gravitating structure has gained renewed attention in recent years with the demonstration that the end products of numerical simulations of cosmological structure formation and dark-matter halos have remarkably universal profiles, in density as well as in pseudo phase-space density, ρ/σ^3. A new aspect, not foreseen by Lynden-Bell's theory or any modifications thereof, is that simulated dark-matter halos appear to have central density cusps, $\rho(r) \sim r^{-1}$, falling to r^{-3} or r^{-4}, or even steeper, in the outer parts (Navarro et al. 1997, 2004; Merritt et al. 2005; Navarro et al. 2010). The origin of such cusps is unclear (see, e.g., Henriksen 2006). There also appears to be a relation between the local density slope and the degree of radial velocity anisotropy (Hansen & Moore 2006).

In this paper, we explore a new avenue for implementing the collisionless nature of dark-matter halos. We suggest to partition state space in energy-per-unit mass shells rather than phase-space elements. Moreover, we implement the corresponding effect of small occupation numbers in this approach. We show that the resulting

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state is a finite-mass system with a cusp, r^{-1}, falling in the outer parts to r^{-4} for a completely relaxed, isolated, isotropic system. This captures the overall properties of simulated halos. In companion papers we compare in detail the resulting states with numerically generated systems suitable for testing our predictions.

2. STATISTICAL MECHANICS

We start out, following Boltzmann (1896) and Ogorodnikov (1957), by defining the number of possible states:

$$W = N! \prod_i \frac{g_i^{n_i}}{n_i!} \tag{1}$$

(as discussed in Section 4 we do not introduce an exclusion principle, cf. Lynden-Bell 1967; Shu 1978; Stiavelli & Bertin 1987). Here, n_i is the occupation number in cell of size g_i in state space (μ space).

It is customary to take the continuous limit ($n_i \to n$), identify $\Gamma(n + 1) = n!$, and optimize $\ln W$ under constraints of fixed total energy and total number of particles using a variational approach. This yields

$$\ln g - \psi(n + 1) = \alpha + \beta E, \tag{2}$$

where $\psi(n) \equiv d \ln \Gamma / dn$ is the digamma function, α and β are Lagrange multipliers associated with the constraints of total number of particles and total energy, respectively, and $E = v^2/2 + \Phi(\mathbf{x})$ is the energy per unit mass, where $\Phi(\mathbf{x})$ is the gravitational potential.

Next, one introduces Stirling's formula

$$\ln n! = \left(n + \frac{1}{2}\right) \ln n - n + \frac{1}{2} \ln(2\pi) + \frac{\theta(n)}{12n} ; \ 0 < \theta(n) < 1 \tag{3}$$

and uses Stirling's approximation for large n

$$\ln n! = n \ln n - n ; \quad n \gg 1 \tag{4}$$

which implies

$$\psi(n + 1) = \ln n ; \quad n \gg 1. \tag{5}$$

This leads to

$$n = g \exp(-\alpha - \beta E). \tag{6}$$

This is the classical finding for the non-degenerate limit, as we did not introduce an exclusion principle in Equation (1). In particular, identifying μ space with the 6-dimensional $(\mathbf{x}, \mathbf{v})$ phase space, the isothermal sphere is retrieved if phase space is divided up equally into equal-size phase-space cells g:

$$f(\mathbf{x}, \mathbf{v}) = A \exp \left(-\beta \left[\frac{1}{2} v^2 + \Phi(\mathbf{x})\right]\right). \tag{7}$$

Below we introduce two modifications to this standard approach, which, combined, give dramatically different structures, which turn out to be reminiscent of the end-products of numerical simulations of collisionless self-gravitating N-body systems.

2.1. *Orbit Space Versus Phase Space*

The first major modification consists in noting that in an equilibrium collisionless system all particles retain their energies. This is not the case in an equilibrium collisional system, such as a classical gas, or a self-gravitating system dominated by two-body encounters, such as a globular cluster. The fundamental property of a collisionless system is that particles are distributed on orbits. In a relaxed system, once an energy is assigned to a particle it stays in a restricted portion of phase space, an energy cell. For an isotropic system, energy is the only isolating integral. Hence, we argue that in partitioning state space, the fundamental partition is energy space, not phase space (see also Efthymiopoulos et al. 2007).

This implies that the occupation number n, Equation (6), should be interpreted as an indicator of the number of particles with a given energy, i.e.,

$$N(E) \propto \exp(-\beta E) \tag{8}$$

and not as the number of particles in a parcel of classical phase space, as is usually assumed.

Binney (1982) (see also, e.g., Hernquist 1990; Spergel & Hernquist 1992; Binney & Tremaine 1987) found that elliptical galaxies obeying the $R^{1/4}$ law have energy distributions very similar to Equation (8), however these authors' motivation for using this form was largely empirical.

Given $N(E)$ one can, of course, recover the classical distribution function. Stiavelli & Bertin (1987) point out that the occupation numbers in the classical phase-space can be related to those in the energy space if the former are assigned non-equal a priori weights, inversely proportional to the volume of phase space with a given energy, i.e.,

$$f(E) \propto g(E)^{-1} \exp(-\beta E), \tag{9}$$

from which Equation (8) is retrieved since $N(E) \equiv f(E)g(E)$ for isotropic systems. The relation between the phase-space density f and the differential energy distribution N is obtained assuming isotropy from $f(\mathbf{x}, \mathbf{v}) d^3\mathbf{v} d^3\mathbf{x} = N(E)dE$ and the density of states $g(E) = d^3\mathbf{v} d^3\mathbf{x}/dE = 16\pi^2 \int_0^{r_{\max}(E)} \sqrt{2(E - \Phi)} r^2 dr$ (Binney & Tremaine 1987).

Another interesting aspect of Equation (8), as pointed out by Binney (1982), is that for systems with less mass at the centers than in the outer parts, β, and hence the effective temperature, $T = \beta^{-1}$, need to be negative (see also Merritt et al. 1989). This is consistent with the self-gravitating nature of the systems, as these are characterized by negative heat capacity (Binney & Tremaine 1987).

2.2. *Small occupation numbers*
2.2.1. *Integer approach*

The second major modification is necessary because in systems with a finite potential depth the occupation numbers in energy cells with very bound energies can become small (Equation (8)). A similar problem is encountered when the classical phase-space distribution function, $f(E)$, takes on an exponential form (Equation (7)), but in this case, because the temperature is positive, the small occupation numbers are found at the near escape energies, i.e., in the outer regions of systems. Madsen (1996) pointed out that in this case the Stirling approximation, Equation (4), breaks down. Following Simons (1994), he argued that the appropriate form for Equation (6) is

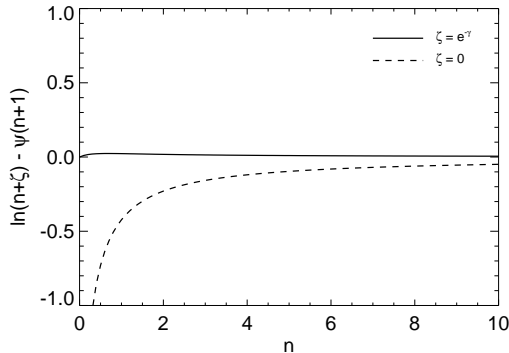$$n_i = [g_i \exp(-\alpha - \beta E_i)], \tag{10}$$

Figure 1. Approximations to $\psi(n+1)$. Comparison of the standard approach ($\zeta = 0$, dashed curve) and the approximation used here ($\zeta = \exp(-\gamma)$, solid curve).

where $[\cdot]$ means rounding down to the nearest integer.

Because the majority of particles in this latter case have energies near escape energies, the small occupation number modification has a dramatic effect on the resulting structures. Madsen (1996) showed that Equation (10) introduces a cutoff which results in finite-mass systems, similar to the King (1966) models of globular clusters. In effect, Madsen (1996) analytically derived the well-known King (1966) models, which were originally obtained as a simple heuristic modification of the isothermal sphere's distribution function, Equation (7).[4]

For collisionless systems, where the temperature is negative, the cutoff occurs at energies close to that of the central potential value, i.e., close to the center of the system. Hence, the effect on the structures is not so dramatic in terms of total mass. But as we show below, it determines the inner density profile of the equilibrium systems.

2.2.2. *Continuous approach*

Because a physical system is not expected to have a step-like differential energy distribution $N(E)$, a continuous version of Equation (10) is needed. We do this by introducing a superior approximation to Stirling's formula which, unlike Equation (5), is not limited to large occupation numbers.

We start by noting that when $n = 0$, one has the exact result $\psi(1) = -\gamma$, where $\gamma \approx 0.57721566...$ is Euler's constant. Combining this with the large n limit, Equation (5) leads to the approximation

$$\psi(n+1) \approx \ln(n + \zeta), \qquad (11)$$

with $\zeta = \exp(-\gamma) \approx 0.561459....$ While simple, this expression is a remarkably good approximation as shown in Figure 1 along with the classical large n approximation (Equation (5); $\zeta = 0$). The deviation from the exact $\psi(n+1)$ is always positive, with a single maximum difference of 0.0237 at $n = 0.680$. Using this in Equation (2), one obtains a modification to Equation (6),

$$n = g \exp(-\alpha - \beta E) - \zeta. \qquad (12)$$

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[4] One can possibly improve upon Madsen (1996)'s Figure 1 by assigning different central potential values of the new models that match the old models. Then, the difference between the two will be confined to low density regions, where it belongs.

Similar modifications have previously been proposed (Landsberg 1954; Hjorth 1993; Menon et al. 2006; Dubey et al. 2008).

The Lagrange multiplier α is determined by requiring that $n = 0$ at some energy E'. Thus, we get

$$n = \zeta(\exp(-\beta[E - E']) - 1), \qquad (13)$$

thereby eliminating the cell size, g, which does not have a unique, physically meaningful value in gravitational systems.

For a system which vanishes at the escape energy, $E' = 0$, and so the classical phase-space occupation number function is $n = \zeta(\exp(-\beta E) - 1)$. The systems we are interested in vanish at a finite central potential, $E' = \Phi_0$, and so the energy-space occupation number function becomes $n = \zeta(\exp(-\beta(E - \Phi_0)) - 1)$. This is the continuous version of Equation (10).

2.3. *DARKexp models*

Equation (13) with $E' = \Phi_0$ incorporates the two modifications we introduced in Sections 2.1 and 2.2. Identifying the occupation number n as being proportional to N, the differential energy distribution, one obtains $N(E) = A(\exp(-\beta[E - \Phi_0]) - 1)$, where A is determined by the mass of the system. In this expression, E and Φ_0 have units of energy, and β is the inverse of temperature. We convert this to dimensionless form, using $\varepsilon = \beta E$ and $\phi_0 = \beta \Phi_0$ (note that both ε and ϕ_0 are positive quantities for bound systems),

$$N(\varepsilon) = A(\exp[\phi_0 - \varepsilon] - 1). \qquad (14)$$

We dub this expression the DARKexp. It represents our prediction for fully relaxed, collisionless, self-gravitating, isotropic systems. Because the arguments presented in this paper do not apply to non-isotropic systems, Equation (14) cannot be directly compared to the results of N-body simulations. Having said that, we note that $N(\varepsilon)$ is not very sensitive to anisotropy, as it depends primarily on the density profile and not on the dynamics of the system.

The detailed structure of the DARKexp systems, including their density and velocity dispersion profiles, will be considered in an accompanying paper (Williams & Hjorth 2010). In the next section, we discuss the limiting behavior of DARKexp models at small and large radii.

3. RESULTING STRUCTURES

3.1. *Limiting Power-Law Behavior at Small Radii*

In a general spherically symmetric structure, the limiting form for the central potential can be assumed to be

$$\phi = \phi_0 - \phi_\alpha r^\alpha + \cdots \qquad (15)$$

Possion's equation $\nabla^2 \phi = 4\pi G \rho$ yields a limiting power-law behavior of the central density,

$$\rho(r) \propto r^{\alpha - 2}. \qquad (16)$$

For $\varepsilon \to \phi_0$ the distribution function then becomes

$$f(\varepsilon) \propto (\phi_0 - \varepsilon)^{-(4+\alpha)/2\alpha} \qquad (17)$$

and the density of states becomes

$$g(\varepsilon) \propto (\phi_0 - \varepsilon)^{(6+\alpha)/2\alpha}. \qquad (18)$$

For similar expressions, see Henriksen & Widrow (1995), Widrow (2000), and Arad et al. (2004). The differential mass distribution $N(\varepsilon) = f(\varepsilon)g(\varepsilon)$ then becomes

$$N(\varepsilon) \propto (\phi_0 - \varepsilon)^{1/\alpha}. \qquad (19)$$

In general, the value of α ranges from 0 for the singular isothermal sphere to $\alpha = 1$ for Navarro–Frenk–White or Hernquist profiles, to shallower slopes, reaching a flat core for $\alpha = 2$. Increasing α corresponds to increasingly steeper $\ln N(\varepsilon)$ versus ε curves. For $\alpha \to \infty$, the system develops a hole in the central density profile, which is unphysical.

3.2. *Limiting Power-Law Behavior at Small Radii for DARKexp Models*

In the DARKexp model, Equation (14), $N(\varepsilon) \propto (\phi_0 - \varepsilon)$ as $\varepsilon \to \phi_0$. In other words, $\alpha = 1$ and we retrieve the central density cusps

$$\rho(r) \propto r^{-1}, \qquad (20)$$

known from numerical simulations. The corresponding distribution function is

$$f(\varepsilon) \propto (\phi_0 - \varepsilon)^{-5/2} \qquad (21)$$

for $\varepsilon \to \phi_0$, which is the same as that of the Hernquist (1990) model.

Thus our proposed differential energy distribution, the DARKexp, naturally predicts that the central density slopes of collisionless self-gravitating systems should asymptote to -1 at the centers of structures. Note that this slope is not the result of any specific dynamical process operating during the formation of halos, but a generic consequence of full relaxation.

The Appendix discusses the limiting behavior for more general cutoffs to $N(\varepsilon) \propto \exp(-\varepsilon)$.

3.3. *Limiting Behavior at Large Radii*

While we are focusing on the inner parts of halos in this paper, we note that a full model for the entire system can be obtained by assuming that $N(\varepsilon)$ is finite at the escape energy and zero above (as plotted in Figure 2). The rationale behind this is that during violent relaxation the escape energy is no special location and $N(\varepsilon)$ is expected to be continuous at what will eventually become the escape energy (Jaffe 1987; Hjorth & Madsen 1991). For such a model $f(\varepsilon) \propto \varepsilon^{5/2}$ and $\rho(r) \propto r^{-4}$ for $\varepsilon \to 0$ and $r \to \infty$, similar to the Hernquist model and broadly consistent with numerical simulations of dark-matter halos. However, if relaxation is not complete at radii where particles have near escape velocities, then the outer density profile slope may deviate from -4.

4. DISCUSSION

4.1. *The approach to equilibrium*

In this paper, we used statistical mechanics to predict the energy distribution function of relaxed systems. A key feature of statistical mechanics approaches is that they deal only with the final equilibrium states, and derive these by equating them to the most probable or maximum entropy states. We stress that our theory is therefore limited to the description of the final state of self-gravitating collisionless systems. Because the final
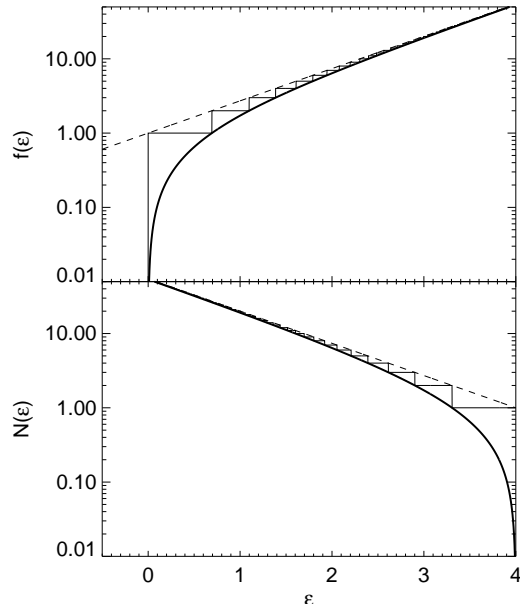

Figure 2. Statistical mechanical predictions for n (Equation (13)). In the usual statistical mechanical approach, one identifies μ space with $(\mathbf{x}, \mathbf{v})$ phase space and n with f (upper panel). In the approach proposed in this paper, one identifies μ space with energy space and n with N (lower panel). We have assumed $\phi_0 = 4$. Different line styles signify different cutoffs: $\zeta = 0$ (no cutoff, thin dashed line), $\zeta = \exp(-\gamma)$ (thick solid curve, DARKexp), and discrete approach (thin solid line, Equation (10)).

state is an equilibrium state, it is the result of full relaxation and therefore does not rely on any additional assumptions.

Implicit in our derivation is the assumption of equal a priori probabilities in state space. While this can be accomplished through efficient mixing (ergodicity), our theory does not address specific physical mechanism for attaining full mixing. In a companion paper (Williams & Hjorth 2010), we use the Extended Secondary Infall Model (ESIM) to test the DARKexp prediction, but stress that ESIM is a restricted physical model and is not equivalent to N-body simulations.

A straightforward way to evaluate the applicability of physical mechanisms for relaxation is to compare their end states. For example, the scattering model for violent relaxation introduced by Spergel & Hernquist (1992) predicts $N(E) \propto [(E - \Phi_0)^{-2} + C(E - \Phi_0)^{-1/2}]^{-1} \exp(-\beta E)$ which is clearly inconsistent with the DARKexp final state. On the other hand, the final state of ESIM halos is well fit with DARKexp.

4.2. *Collisional Versus Collisionless Systems*

Our prediction for $N(\varepsilon)$ applies to the end states of collisionless dynamics. Collisionlessness has several different consequences, many of which can be used in one's theory. Lynden-Bell (1967) used the collisionless Boltzmann equation to introduce an exclusion principle to account for the incompressibility of the phase-space fluid. We use a different property; that collisionless dynamics implies the constancy of the energy per unit mass for each particle. Therefore, the collisionless nature of the problem is automatically included and there is no need for an exclusion principle.

In a system driven toward equilibrium by two-body relaxation, the situation is quite different. In this case, efficient relaxation implies that any particle can in principle end up anywhere in phase space and the usual partition of μ space is appropriate. In this case, taking into account low occupation numbers, one retrieves the King (1966) $f(E)$ which is rounded down at near escape energies, while DARKexp's collisionless $N(E)$ is rounded down at highly bound energies.

The density profiles of the two are clearly different, but both are very good approximations to what one sees in globular clusters and simulated dark-matter haloes, respectively.

4.3. Anisotropy

In this paper we dealt exclusively with isotropic systems for which the differential energy distribution is a function of energy only. The full simulated structures, however, are definitely anisotropic, and exhibit a correlation between the density slope and anisotropy (Hansen & Moore 2006).

In principle, our statistical mechanics formalism can be extended to spherical non-isotropic systems, and we plan to do so in a future publication. In a fully developed theory, the distribution function must depend explicitly on angular momentum, especially in the outer parts (e.g., Stiavelli & Bertin 1987). Whether the energy distribution of the full theory will be significantly affected by the introduction of angular momentum is yet unclear; numerical experiments of MacMillan et al. (2006, Figure 9) seem to indicate that the DARKexp form is still a good description of systems that underwent radial orbit instability.

For now we note that even though the DARKexp prediction may not be expected to be an excellent fit to simulations at all energies, it should apply to the central regions of dark-matter halos, as these are isotropic. Therefore, our explanation of the central density cusp of -1 applies to simulated halos.

APPENDIX

LIMITING BEHAVIOR AT SMALL RADII FOR DIFFERENT EXPONENTIAL CUTOFFS

One might accept that $N(\varepsilon) \propto \exp(-\varepsilon)$ (Section 2.1), but not the proposed form of the cutoff motivated by the low occupation numbers (Section 2.2), for example, because our proposed transition from the integer to the continuous form is more algebraic than physical. In this section we address possible alternatives to the cutoff shape.

First, is a cutoff needed at all? If there is no cutoff, then the differential energy distribution is of the form Equation (8), which would lead to a singularity in the central potential. To avoid that, one needs a cutoff. One possible form is to simply truncate $N(\varepsilon)$ at some finite central value; $N(\varepsilon) = C$ at $\varepsilon = \phi_0$ and $N(\varepsilon) = 0$ for $\varepsilon > \phi_0$. This would imply $\alpha = \infty$, and an infinite, positive central density slope, i.e., a hole (Section 3.1) and divergent velocity dispersion, both of which are unphysical.

Therefore, we conclude that a smooth cutoff is required, i.e., that at some finite ϕ_0, $N(\varepsilon = \phi_0) = 0$. At energies near these highly bound energies, we can Taylor expand the non-truncated $N(\varepsilon)$. Using the abbreviation, $x = \phi_0 - \varepsilon$: $\exp(x) \sim 1 + x + x^2/2 + \cdots$. Whatever the specific shape of the cutoff function, it too can be Taylor expanded, and then subtracted from that of $\exp(x)$. Three outcomes can result after this subtraction, depending on the exponent of x of the surviving leading term, (1) x^B, where $B < 1$ and x and higher terms cancel out; (2) x; and (3) x^2, if the cutoff function goes exactly as $1 + x$. In case (1) $\alpha > 1$, and the central density slope will be shallower than -1. Case (2) leads to our main prediction of the central density slope of -1, while case (3) is the only way to get density slopes steeper than -1. In this case $\alpha = 0.5$, and the central density slope is -1.5.

Since mathematically it is possible to get central density slopes shallower or steeper than -1, it is ultimately the physical arguments that will dictate the form of the cutoff in $N(\varepsilon)$ and hence the slope value.

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